

# Quantum mechanical implementation of DNA algorithm for satisfiability problem

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## Abstract

DNA computation could in principle solve the satisfiability (SAT) problem due to the operations in parallel on extremely large numbers of strands. We demonstrate some quantum gates corresponding to the DNA ones, based on which an implementation of DNA algorithm for SAT problem is available by quantum mechanical way. Since quantum computation owns the favorable feature of operations in parallel on  $2^n$  states by using only  $n$  qubits, instead of  $2^n$  strands in DNA computation, computational complexity is much reduced in treating the SAT problem quantum mechanically. We take a three-clause SAT problem with two variables as an example, and carry out a NMR experiment for solving a one-variable SAT problem.

PACS numbers: 03.67.Ac, 89.70.Eg, 87.14.gk, 87.10.Tf

Recent years have witnessed some outstanding breakthroughs in the molecular computation proposed by Feynman [1] in 1961. For example, one of the famous non-deterministic polynomial (NP) problems, i.e., satisfiability (SAT) problem, has been in principle worked out by biological computation with DNA strands [2, 3]. As it is generally considered that other NP problems could be reduced to a solvable SAT problem [4], the achieved solutions by the DNA-based biological computation (DNAC) present us hopes to solve all the NP problems.

On the other hand, quantum computation (QC), another proposal by Feynman [5], has drawn much attention over past decades. Eight atomic qubits [6] and six photonic qubits [7] have been entangled so far, respectively, and simple quantum algorithms have been tested experimentally [8]. It is believed that QC outperforms classical computation in treating some NP problems [9, 10, 11, 12, 13].

DNAC could potentially have vastly more parallelism than conventional classical computations, which makes it possible to solve the SAT problem in principle. In contrast, QC, running in an intrinsically different mechanism, works on qubits which would be encoded in states  $|0\rangle$  and  $|1\rangle$  as well as in arbitrary superposition of  $|0\rangle$  and  $|1\rangle$ . As a result, the computation in parallelism in QC could be done naturally by superposition of states in a single system. Therefore, to represent  $2^n$  states, we need  $2^n$  DNA strands in computation, but only  $n$  qubits quantum mechanically. Besides, entanglement is the unique feature in QC, which is the base of quantum logic gates and related to nonlocality. Another feature of QC, different from DNAC, is the state collapse due to measurement. To keep a qubit unchanged after measurement, we have to employ auxiliary qubits.

The present work focuses on finding some relations between DNAC and QC, based on which the solution of the SAT problem by DNAC algorithm would be carried out quantum mechanically. As a parallel implementing computation, DNAC could in principle solve a SAT problem with extremely large number of strands (i.e., bits). In contrast, the QC, running on much less resource of qubits, should be able to solve the same problem much more efficiently even following the same computing route. So once we could find the correspondence between the basic operations of DNAC and QC, a translation of the DNA algorithm to quantum version will make us available to try a quantum mechanical implementation of DNA algorithm. We argue that it would help us find new functions of QC and new ways to quantum algorithm even if such a DNAC-based quantum mechanical implementation would

not really reduce NP problems to P problems. On the other hand, DNAC would be further understood from our study with QC. We will also test our quantum treatment by Nuclear Magnetic Resonance (NMR) experiment.

We first review briefly the basic operations in DNAC [15]: *Append*, *Extract*, *Discard*, *Amplify*, *Merge*, *Detect* and *Read*. The operation *Append*, including *Append – Head* and *Append – Tail*, is to put a short DNA strand to the head and the tail of a long strand, respectively. That is to say, *Append – Head*( $B, u_j$ ) =  $\{u_j, B_n, B_{n-1}, \dots, B_2, B_1\}$ , and *Append – Tail*( $B, u_j$ ) =  $\{B_n, B_{n-1}, \dots, B_2, B_1, u_j\}$ , with  $B$  a set consisting of a number of elements  $B_k$  ( $k = 1, \dots, n$ ). *Extract* is to extract some of the required DNA strands. In most operations, *Extract* results in a separation of one tube into two with one tube involving the required strands and the other involving the rest. The corresponding formulas are  $+ \{U, u_j^1\} = \{u_n, u_{n-1}, \dots, u_j^1, \dots, u_2, u_1\}$  and  $- \{U, u_j^1\} = \{u_n, u_{n-1}, \dots, u_j^0, \dots, u_2, u_1\}$  with  $U$  the set involving elements  $u_k$  ( $k = 1, \dots, n$ ) and  $u_j^1$  and  $u_j^0$  denoting values of  $u_j$  to be 1 and 0, respectively. *Discard* is to null a tube, i.e., removing each DNA strand from the tube. *Amplify* replicates all of the DNA strands in the test tube, which creates a number of identical copies and then *Discard* the original one. *Merge* corresponds to the operation to pour many tubes of DNA strands into one tube without any change in the individual strands, which could be described by  $\cup(P_1, P_2, \dots, P_n) = P_1 \cup P_2 \cup \dots \cup P_n$ , with  $P_k$  ( $k = 1, 2, \dots, n$ ) being a tube with DNA stands. *Detect* leads to a result 'YES' once there is at least one DNA strand in the tube, or 'NO' otherwise. *Read* gives an explicit description of one DNA strand no matter how many molecules in the tube.

On the side of QC, there are some basic operations constituting universal QC [16], where the most frequently mentioned gates are  $\mathbf{R}(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$  for the qubit encoding  $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , Hadamard gate  $\mathbf{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$  to change  $|0\rangle$  to  $(|0\rangle + |1\rangle)/\sqrt{2}$  and  $|1\rangle$  to  $(|0\rangle - |1\rangle)/\sqrt{2}$ , and controlled-NOT gate  $\mathbf{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ . To be more efficient, we sometimes employ three-qubit Toffoli gate  $\mathbf{TOFF}$  to flip the target qubit when the two

control qubits are both in states  $|1\rangle$ .

Comparing QC with DNAC, we could find some relations between them. Quantum mechanically, *Append* could be described as a tensor product, i.e.,  $Append - Head(B, u_j) = \{u_j\} \otimes \{B\}$  and  $Append - Tail(B, u_j) = \{B\} \otimes \{u_j\}$ . The operation *Extract* could, to some extent, be carried out by **CNOT**. On the other hand, a Hadamard gate in QC could be carried out by the operations of DNAC with *Extract* to separate two subsets respectively including  $|0\rangle$  and  $|1\rangle$ , and then with *Append* and *Merge* to realize  $|0\rangle \rightarrow (|0\rangle + |1\rangle)/\sqrt{2}$  and  $|1\rangle \rightarrow (|0\rangle - |1\rangle)/\sqrt{2}$ . To be specific, we give an example below to simulate quantum superposition by operations in DNAC. We initially have an empty set  $\{\phi\}$ , and replicate it by *Amplify* $\{\phi\}$  to be two empty sets.  $Append - Tail\{\phi, |0\rangle\}$  and  $Append - Tail\{\phi, |1\rangle\}$  yield the sets  $\{|0\rangle\}$  and  $\{|1\rangle\}$ , respectively. After the operation *Merge*, we could have a superposition in the set  $\{|0\rangle + |1\rangle\}$ , equivalent to  $\mathbf{H}|0\rangle$  in QC. Repeating above steps, we could also get the set  $\{(|0\rangle + |1\rangle)|0\rangle + (|0\rangle + |1\rangle)|1\rangle\}$ , actually corresponding to  $\mathbf{H}|0\rangle \otimes \mathbf{H}|0\rangle$  in QC. Nevertheless, it seems that DNAC could not fully accomplish the jobs by QC. For example, the QC operation  $\mathbf{R}(\theta)$  with  $0 < \theta < 2\pi$  could not be efficiently simulated by DNAC. But QC could carry out any job by DNAC in a more efficient way.

In what follows, we will solve a SAT problem quantum mechanically following the route in DNAC. As mentioned above, QC using qubits could save the resource from  $2^n$  DNA strands to  $n$  qubits. Even if there are auxiliary qubits involved, the number of qubits increases only linearly with the size of the QC task. Let's consider a simple case as an example with the formula

$$F = (u_2 \vee u_1) \wedge (\overline{u_2} \vee \overline{u_1}) \wedge (u_1), \quad (1)$$

where  $u_2$  and  $u_1$  are Boolean variables whose values can be 0 (false) or 1 (True).  $\vee$  is the “logical OR” operation with  $u_2 \vee u_1 = 0$  only if  $u_2 = u_1 = 0$ , and  $\wedge$  is the “logical AND” operation with  $u_2 \wedge u_1 = 1$  only if  $u_2 = u_1 = 1$ .  $\overline{u_2}$  and  $\overline{u_1}$  are the operations “NEGATION” of  $u_2$  and  $u_1$ , respectively, i.e.,  $\overline{u_2}$  being 0 if  $u_2 = 1$  and being 1 if  $u_2 = 0$ . The satisfiability problem is to find appropriate values for  $u_2$  and  $u_1$  to make the formula  $F$  true.

The logic AND and OR could be carried out by quantum circuits [17], as shown in Fig. 1. To solve Eq. (1), we employ four quantum registers  $|u_2u_1\rangle$ ,  $|y_2y_1\rangle$ ,  $|r_2r_1r_0\rangle$  and  $|c_3c_2c_1c_0\rangle$ , which are introduced basically from the idea of DNAC [3].  $u_2$  and  $u_1$  are qubits initially zero and then in superposition by Hadamard gates.  $y_2$  and  $y_1$ , also initially being zero, are auxiliary qubits acting as copies of  $u_2$  and  $u_1$ , respectively. The third register stores

the results of OR, where the qubits inside are initially prepared to be  $r_2^1$ ,  $r_1^1$ , and  $r_0^0$ , with the superscripts being values of the qubits. After each time with the data transferred to the third register from the second one,  $y_2$  and  $y_1$  will be nulled for later use. The fourth register, including four qubits, are used for storing the results of AND, where except  $|c_0^1\rangle$ , other qubits are initially zero. After each AND operation, the results are stored in  $|c_3\rangle$ ,  $|c_2\rangle$ , or  $|c_1\rangle$ , respectively, and we have to restore the qubits in the third register to be  $r_2^1$ ,  $r_1^1$ , and  $r_0^0$  for later use repeatedly. With these ideas, to accomplish an evaluation of Eq. (1), we design a quantum circuit in Fig. 2, where the qubits are input from the left-hand side of the circuit. We get started from the input state  $|u_2^0 u_1^0\rangle |y_2^0 y_1^0\rangle |r_2^1 r_1^1 r_0^0\rangle |c_3^0 c_2^0 c_1^0 c_0^1\rangle$ . Following the gates in Fig. 2 step by step, we finally obtain, after a measurement on  $|c_3^1\rangle$ ,  $|u_2^0 u_1^1\rangle |y_2^0 y_1^0\rangle |r_2^1 r_1^1 r_0^0\rangle |c_2^1 c_1^1 c_0^1\rangle$ , implying the correct values of  $u_2$  and  $u_1$  to be 0 and 1, respectively.

We will below employ NMR approach to check our theory experimentally. Although the quantum information processed by NMR is made on the ensemble of nuclear spins, instead of individual spins, NMR has remained to be the most convenient experimental tool to demonstrate quantum information processing due to its mature and well-controllable technology [18]. We will employ spatial averaging method [19] to prepare the thermal equilibrium ensemble to the pseudo-pure state. To make the experimental operations simple and reliable, we will carry out below a three-qubit case corresponding to a solution of the simplest SAT problem  $F = (u_1)$ , i.e., a SAT with one clause involving only a single variable. The quantum circuit is plotted in Fig. 3, where  $|u_1\rangle$  is the qubit holding the variable,  $|y_1\rangle$  is the copy of  $|u_1\rangle$ , and  $|c_1\rangle$  is to store the evaluating result. Following the steps in Fig. 3, we could obtain the output  $(|000\rangle + |101\rangle)/\sqrt{2}$ . By a measurement on  $|c_1^1\rangle$ , we could obtain  $|u_1^1\rangle$  and  $|y_1^0\rangle$ , which means that the evaluation of  $u_1$  should be one and  $y_1$  has been nulled for later use.

We have carried out the quantum circuit experimentally on a Varian INOVA 500 NMR spectrometer with the sample  $^{13}\text{C}$ -labelled alanine, i.e.,  $^{13}_1\text{CH}_3 - ^{13}_2\text{CH}(\text{NH}_2) - ^{13}_3\text{COOH}$ . The three qubits are encoded in the carbons  $^{13}_1\text{C}$ ,  $^{13}_2\text{C}$ ,  $^{13}_3\text{C}$ , respectively, with  $J$ -coupling constants  $J_{12} = 34.79$  Hz,  $J_{23} = 54.01$  Hz, and  $J_{13} = 1.20$  Hz. The pulse sequences to prepare the pseudo-pure state are from [14]. The Hadamard gate can be realized by a single  $\pi/2$  pulse along the  $x$  axis and **CNOT** is implemented by the pulses [19]  $[\pi/2]_y^2 \rightarrow (1/4J) \rightarrow [\pi]_x^{1,2} \rightarrow (1/4J) \rightarrow [\pi]_x^{1,2} \rightarrow [\pi/2]_x^2$ . However, due to weak measurement in NMR, we have no state collapse after a measurement. Besides, only single quantum coherence can be detected

in NMR. As a result, we have to employ some additional operations for detecting the output state  $(|000\rangle + |101\rangle)/\sqrt{2}$ . We may detect the second qubit directly by applying a  $\pi/2$  readout pulse along the  $x$  axis, yielding Fig. 4(b). But for the first and third qubits, we need to disentangle them before measurement. To this end, we apply a **CNOT** gate, respectively, on the first and second qubits followed by another **CNOT** gate, respectively, on the second and first qubits to get the state  $(|000\rangle + |011\rangle)/\sqrt{2}$ . Then the first qubit can be read out by a single  $\pi/2$  pulse along the  $x$  axis, as shown in Fig. 4(a). Similar steps applied to the third qubit result in the spectrum in Fig. 4(c).

The experimental results are in good agreement with our theoretical prediction, which proves the SAT problem to be solvable by QC. Some remarks must be addressed. First of all, the three-qubit NMR experiment we have carried out suffices to make a comprehensive test for our theory, because we have achieved the key aspects of our theory. Although the simple cases with eleven and three qubits, respectively, did not reflect the efficiency of QC implementation for SAT problem, we argue that, with more variables and clauses involved, the QC efficiency would be more and more evident, which could also be found in our later discussion about the computational complexity. Secondly, DNAC does not involve entanglement, whereas entanglement does appear in our quantum treatment. The necessity of additional operations to disentangle the output qubits is not the intrinsic characteristic of our quantum mechanical treatment, but due to the unique feature of NMR technique. Anyway, those additional operations have not changed the essence of our implementation. Thirdly, although it is workable in solving SAT problems, DNAC has been lack of mathematical description. In this sense, our investigation of the relation between DNAC and QC actually presents a mathematical description of the DNAC operations, which is helpful for us to further understand the efficiency and the functions of DNAC.

It is very difficult to discover a quantum algorithm with exponential speed-up. That is why the frequently mentioned quantum algorithms have been only few so far. We argue that, even if it does not provide a general way to reduction of the NP problem to a P problem, our quantum version of the DNAC algorithm should be able to efficiently reduce the computational complexity, compared to the original DNAC treatment. We have simply assessed the computational complexity of our quantum treatment from Fig. 2 and more general consideration for the SAT problem with  $m$  clauses and  $n$  variables [20]: The time complexity is  $O(n)$  **H** gates,  $O(6 \times m \times n)$  **NOT** gates,  $O(2 \times m \times n)$  **CNOT** gates,

$O(m \times n + m)$  **TOFF** gates, and  $O(1)$  projective operations for measurement. The space complexity is  $O(m + 3 \times n + 2)$  qubits, involving the qubits for ancillary. More strict proof in detail will be published elsewhere.

In summary, we have demonstrated a quantum mechanical implementation of DNAC to solve a SAT problem. Both QC and DNAC are hot topics as interdisciplinary subjects, and both of them have merits and drawbacks [2, 3, 21]. Our investigation has presented the relations between them, and we argue that quantum treatment could reduce the complexity of the solution to some NP problems. The relations we have presented between QC and DNAC could enable not only a further exploration of new ways to QC algorithm, but also a further understanding of DNAC from a brand-new angle.

The work is partly supported by NNSFC under Grant No. 10774163, by NFRPC under Grant No 2006CB921203, and partly by NSC under Grants No. 96-2221-E-151-008- and 96-2218-E-151-004-.

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### Captions of the Figures

**Fig. 1** Quantum circuits for (a) the operation AND, i.e., a three-qubit **TOFF** gate, and (b) the operation OR with a three-qubit **TOFF** gate sandwiched by four **NOT** gates, where the wide black side means the output side.

**Fig. 2** Quantum circuits with eleven qubits for solving a three-clause SAT problem with two variables, where some of the registers hold qubits and some for auxiliary qubits, as explained in the text. The superscript 0 or 1 means the initial value of the register.

**Fig. 3** Quantum circuit for solving  $F = (u_1)$ , where the measurement is made on the third (i.e., the bottom) qubit. But due to the unique feature of NMR, we need additional gates in our experiment for the readout of each qubit.

**Fig. 4** NMR experimental spectra for qubit outputs of solution to  $F = (u_1)$ , where the plots from the top to bottom correspond to (a), (b) and (c) for the outputs regarding the first, second and third registers, respectively.